In [1]:
```
#Import Required Libraries
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score, classification_report
import matplotlib.pyplot as plt
import seaborn as sns
```

In [3]:
```
#Load the dataset
Lipinski = pd.read_csv("C:\Lipinski.csv")
Lipinski.head()
```

Out[3]:

	Name	Molecular_Weight	XLogP	H-Bond_Donor_Count	H-Bond_Acceptor_Count	
0	Glycyrrhizin	822.9	3.7	8	16	
1	Etoposide	588.6	0.6	3	13	
2	Vinblastine	811.0	3.7	3	12	(
3	Vincristine	825.0	2.8	3	12	C
4	Sorafenib	464.8	4.1	3	7	CN

In [4]:
```
#Display dataset structure including columns,dtypes,and non-null values
Lipinski.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 160 entries, 0 to 159
Data columns (total 6 columns):
 #   Column                 Non-Null Count  Dtype  
---  ------                 --------------  -----  
 0   Name                   160 non-null    object 
 1   Molecular_Weight       160 non-null    float64
 2   XLogP                  160 non-null    float64
 3   H-Bond_Donor_Count     160 non-null    int64  
 4   H-Bond_Acceptor_Count  160 non-null    int64  
 5   SMILES                 160 non-null    object 
dtypes: float64(2), int64(2), object(2)
memory usage: 7.6+ KB
```

In [5]:
```
#Show the names of all available columns
print(Lipinski.columns)
```

```
Index(['Name', 'Molecular_Weight', 'XLogP', 'H-Bond_Donor_Count',
       'H-Bond_Acceptor_Count', 'SMILES'],
      dtype='object')
```

In [6]:
```
#Drop columns that are not relevant for lipinski rule analysis
Lipinski = Lipinski.drop(columns=['Name', 'SMILES'])
print(Lipinski.columns)
```

```
Index(['Molecular_Weight', 'XLogP', 'H-Bond_Donor_Count',
       'H-Bond_Acceptor_Count'],
      dtype='object')
```

In [7]:
```
# Applying lipinski's rule of 5
# Returns 1 for Drug-like (0 or 1 violations), 0 for Non-drug-like (more than 1 v
def Lipinski_rule(row):
    molecular_weight = row['Molecular_Weight']
    xlogp = row['XLogP']
    h_bond_donors = row['H-Bond_Donor_Count']
    h_bond_acceptors = row['H-Bond_Acceptor_Count']

    violations = 0

    if molecular_weight > 500:
        violations += 1
    if xlogp > 5:
        violations += 1
    if h_bond_donors > 5:
        violations += 1
    if h_bond_acceptors > 10:
        violations += 1

    if violations > 1:
        return 0
    else:
        return 1
```

In [8]:
```
#Add 'Target' column to classify compounds for machine learning
Lipinski['Target']=Lipinski.apply(Lipinski_rule,axis=1)
print(Lipinski)
```

```
     Molecular_Weight  XLogP  H-Bond_Donor_Count  H-Bond_Acceptor_Count  \
0               822.9    3.7                   8                     16
1               588.6    0.6                   3                     13
2               811.0    3.7                   3                     12
3               825.0    2.8                   3                     12
4               464.8    4.1                   3                      7
..                ...    ...                 ...                    ...
155             572.7    3.5                   4                      7
156             588.5    1.4                   9                     14
157             684.6   -1.1                   7                     17
158             404.4   -0.4                   6                     10
159             586.6    2.2                   5                     11

     Target
0         0
1         0
2         0
3         0
4         1
..      ...
155       1
156       0
157       0
158       1
159       0

[160 rows x 5 columns]
```

In [9]:
```
# Check distribution of drug-like (1) and non-drug-like (0) compounds
Lipinski['Target'].value_counts()
```

Out[9]:
```
Target
1    103
0     57
Name: count, dtype: int64
```

In [10]:
```python
# Separate features (X) and target labels (y) for machine learning
X = Lipinski[['Molecular_Weight', 'XLogP', 'H-Bond_Donor_Count',
       'H-Bond_Acceptor_Count']]
y = Lipinski['Target']
```

In [11]:
```python
Lipinski.shape
```

Out[11]:
```
(160, 5)
```

In [12]:
```python
# Split the dataset into training and testing sets for model evaluation
train, test = train_test_split(Lipinski, test_size = 0.3)
print(train.shape)
print(test.shape)
```

```
(112, 5)
(48, 5)
```

In [13]:
```python
train_X = train[['Molecular_Weight', 'XLogP', 'H-Bond_Donor_Count',
       'H-Bond_Acceptor_Count']]
train_y=train.Target
test_X= test[['Molecular_Weight', 'XLogP', 'H-Bond_Donor_Count',
       'H-Bond_Acceptor_Count']]
test_y =test.Target
```

In [14]:
```python
train_X.head(5)
```

Out[14]:

	Molecular_Weight	XLogP	H-Bond_Donor_Count	H-Bond_Acceptor_Count
132	420.6	3.8	3	6
110	435.4	-0.8	4	10
26	522.6	2.0	4	12
30	520.5	2.9	4	9
52	430.9	4.2	3	7

In [15]:
```python
test_X.head(5)
```

Out[15]:

	Molecular_Weight	XLogP	H-Bond_Donor_Count	H-Bond_Acceptor_Count
4	464.8	4.1	3	7
57	619.7	5.1	3	10
102	411.4	2.0	5	8
129	404.9	2.1	3	5
154	581.6	5.2	3	11

In [16]:
```python
train_y.head()
```

Out[16]:
```
132    1
110    1
26     0
30     1
52     1
Name: Target, dtype: int64
```

In [32]:
```python
# Train Logistic Regression, SVM, Decision Tree, and KNN models and evaluate their
model = LogisticRegression()
model.fit(train_X,train_y)
prediction=model.predict(test_X)
print('The accuracy of the Logistic Regression is',accuracy_score(prediction,test_
```

```
The accuracy of the Logistic Regression is 0.9166666666666666
```

In [33]:
```python
from sklearn.svm import SVC
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
```

In [34]:
```python
model = SVC(kernel= 'linear')
model.fit(train_X,train_y)
prediction=model.predict(test_X)
print('The accuracy of the SVM is',accuracy_score(prediction,test_y))
```

```
The accuracy of the SVM is 0.8958333333333334
```

In [35]:
```python
model = DecisionTreeClassifier()
model.fit(train_X,train_y)
prediction=model.predict(test_X)
print('The accuracy of the Decision Tree is',accuracy_score(prediction,test_y))
```

```
The accuracy of the Decision Tree is 0.9583333333333334
```

In [36]:
```python
model = KNeighborsClassifier(n_neighbors= 3)
model.fit(train_X,train_y)
prediction=model.predict(test_X)
print('The accuracy of the KNN is',accuracy_score(prediction,test_y))
```

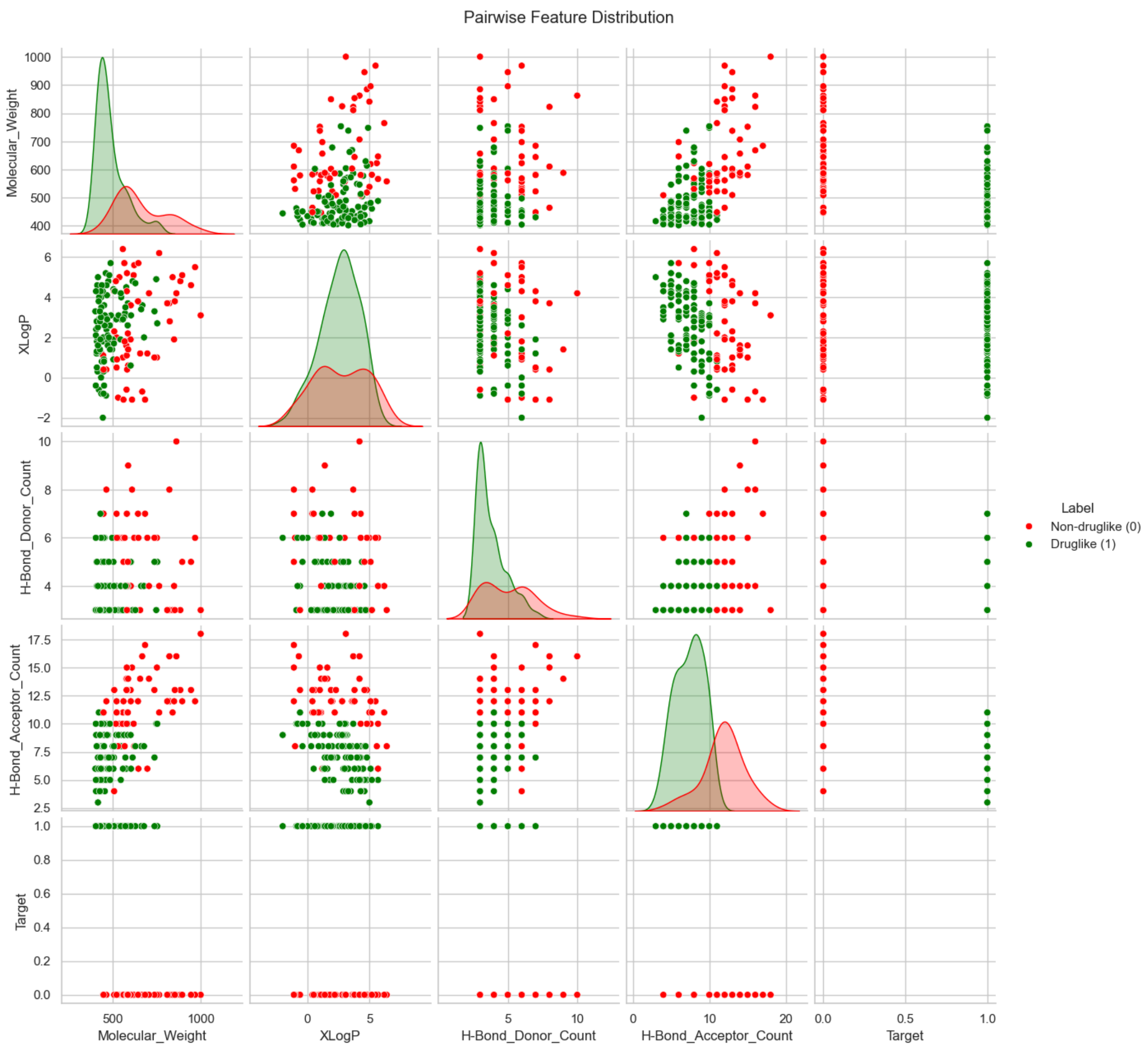
```
The accuracy of the KNN is 0.75
```

In [37]:
```python
#Visualization
sns.set(style='whitegrid')
```

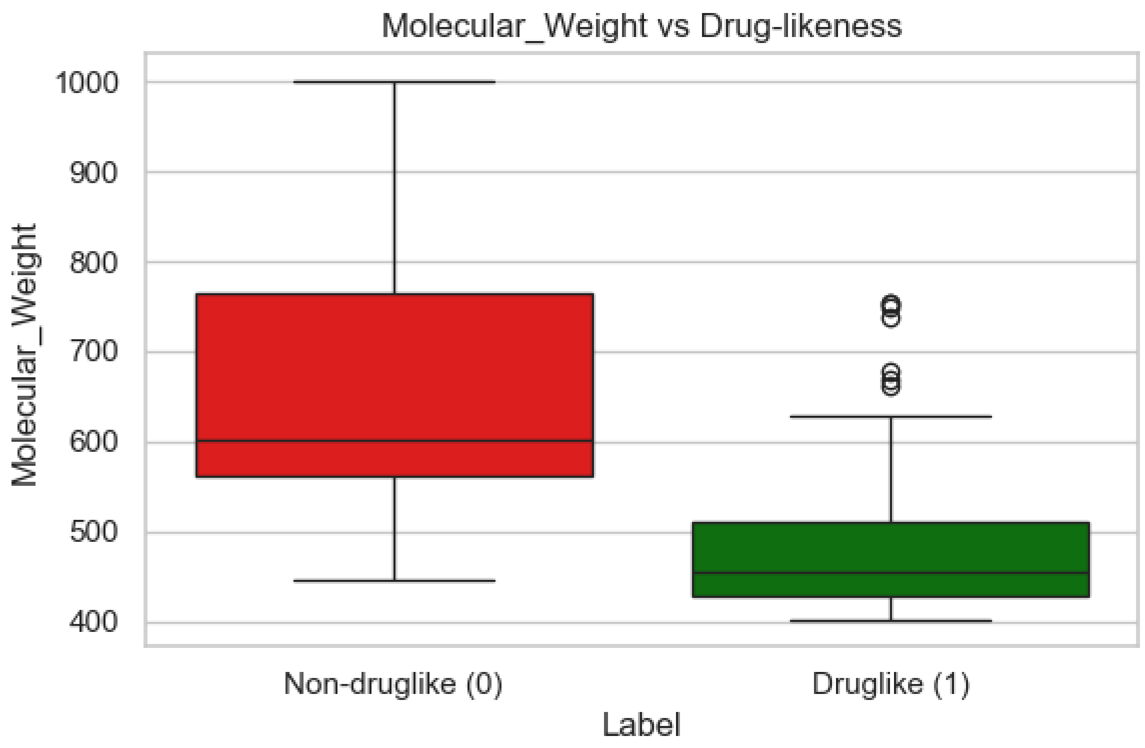
In [26]:
```python
Lipinski['Label'] = Lipinski['Target'].map({1: 'Druglike (1)', 0: 'Non-druglike (
```

In [27]:
```python
palette = {'Druglike (1)': 'green', 'Non-druglike (0)': 'red'}
```

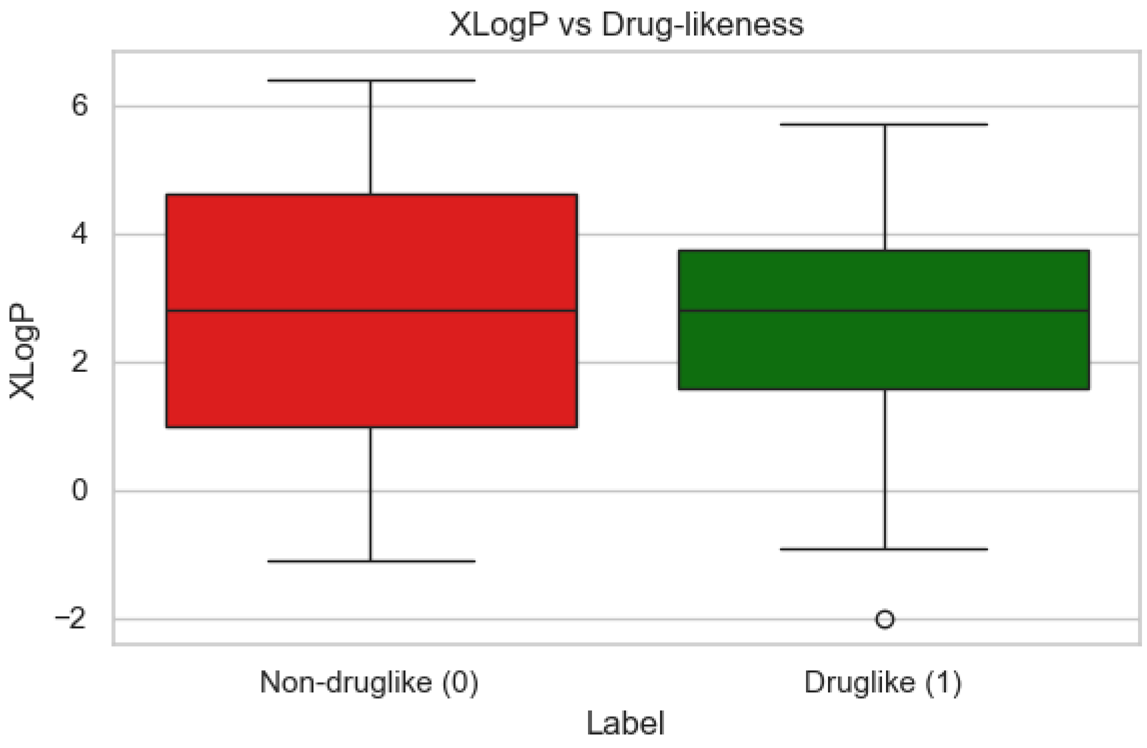
In [28]:
```python
# Visualize pairwise relationships between features using seaborn pairplot
sns.pairplot(Lipinski, hue='Label', palette=palette)
plt.suptitle("Pairwise Feature Distribution", y=1.02)
plt.show()
```



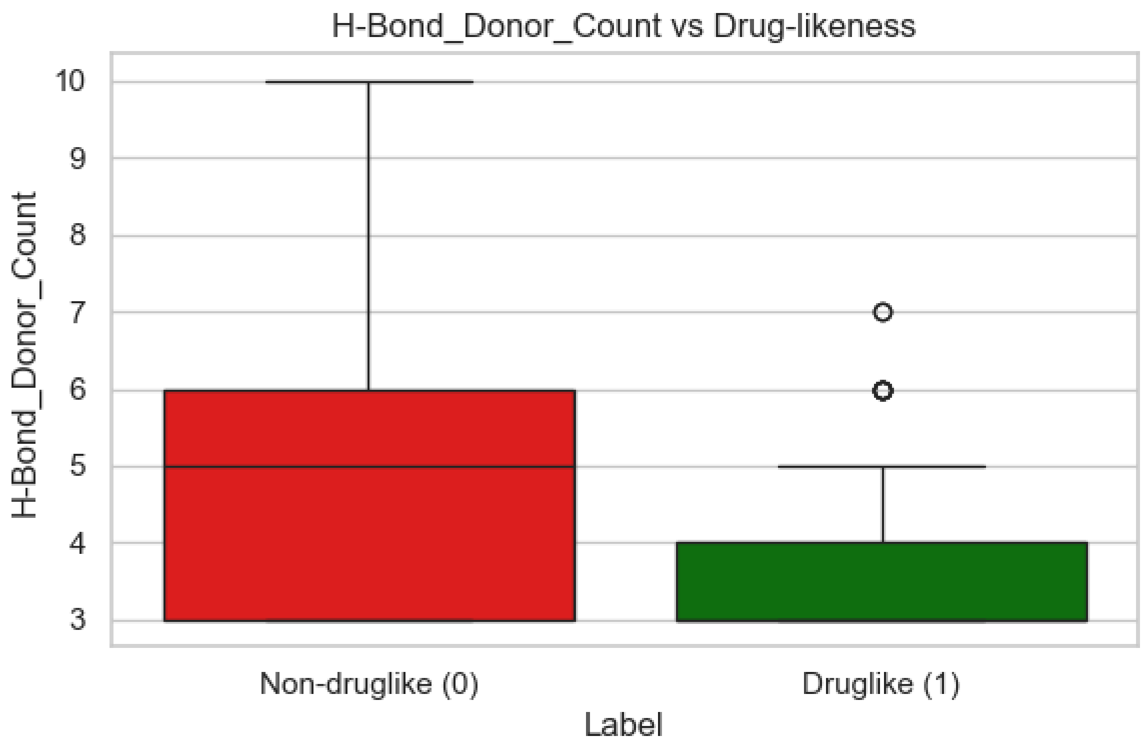
```
In [29]: # Show distribution and outliers using a boxplot
         features = ['Molecular_Weight', 'XLogP', 'H-Bond_Donor_Count', 'H-Bond_Acceptor_Co

         for feature in features:
             plt.figure(figsize=(6, 4))
             sns.boxplot(x='Label', y=feature, data=Lipinski, hue='Label', palette=palette)
             plt.title(f"{feature} vs Drug-likeness")
             plt.tight_layout()
             plt.show()
```

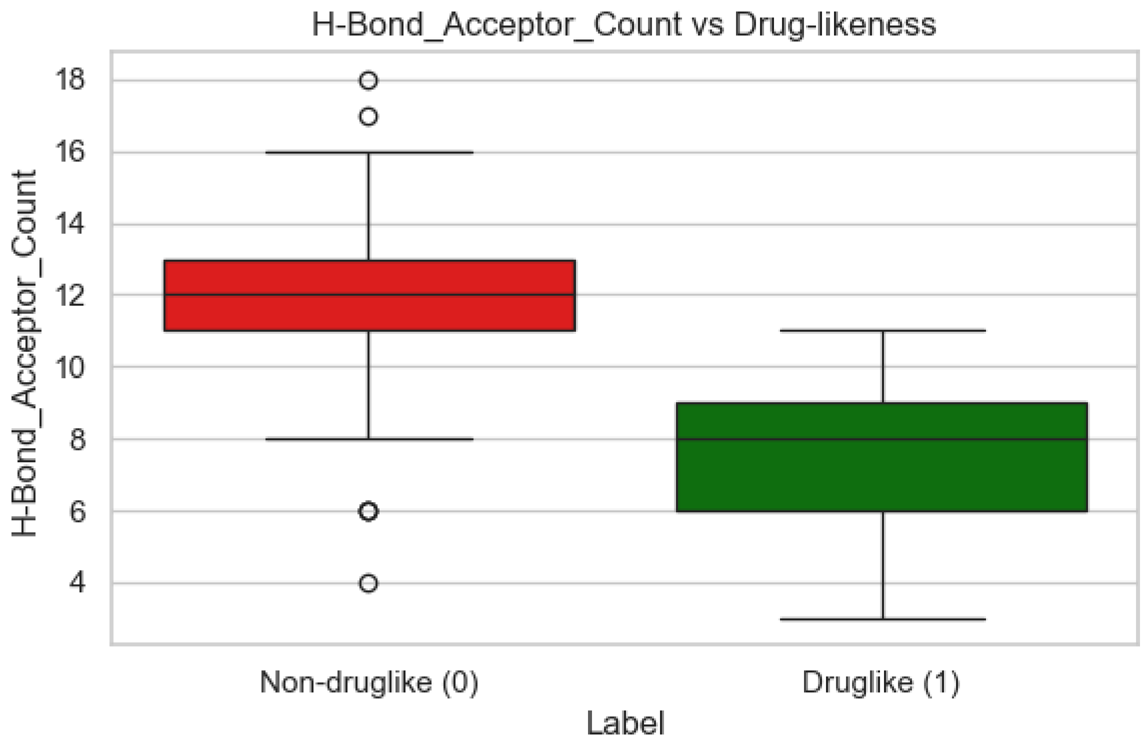


Molecular_Weight vs Drug-likeness
1000
900
800
700
600
500
400
Molecular_Weight
Non-druglike (0)
Druglike (1)
Label



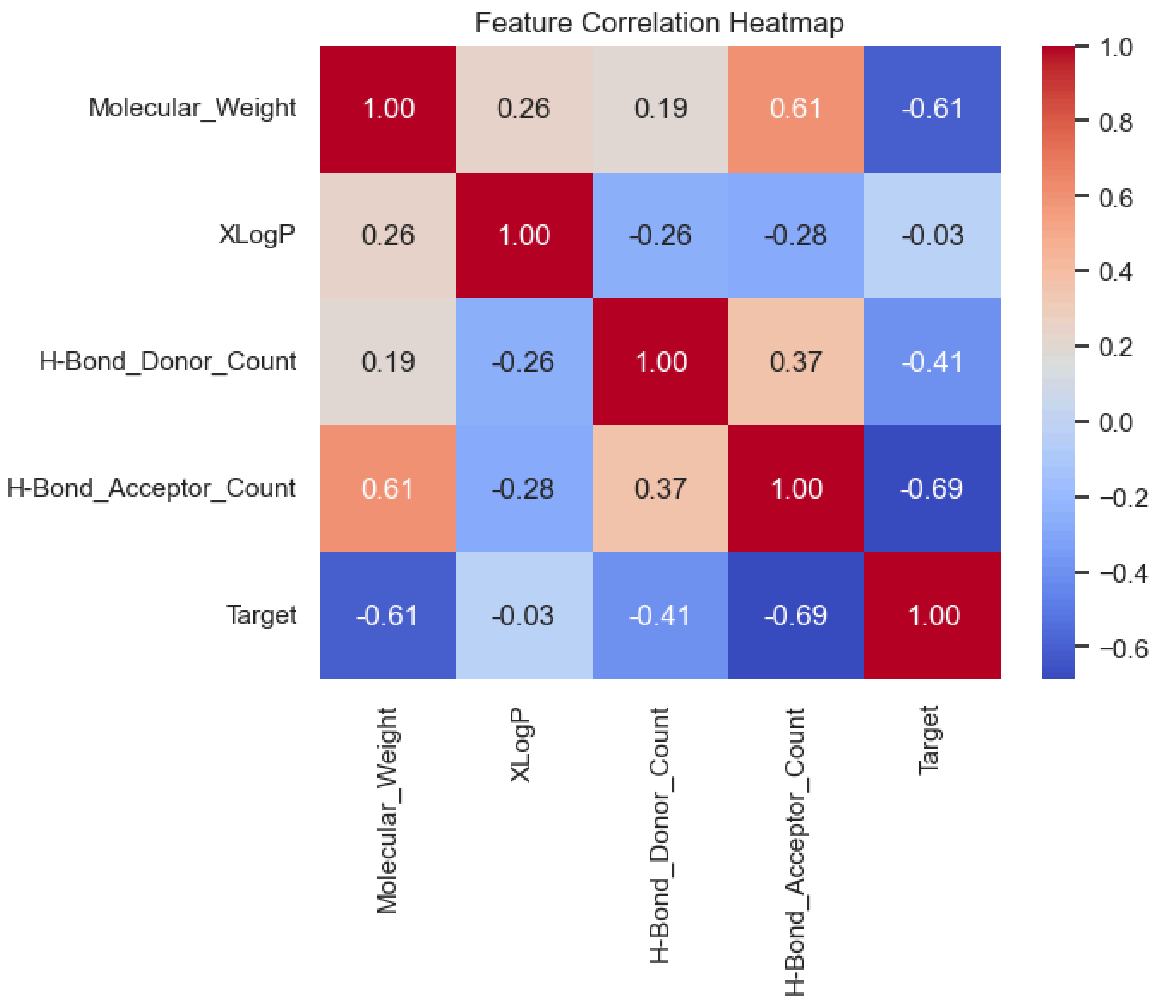
XLogP vs Drug-likeness
6
4
2
0
−2
XLogP
Non-druglike (0)
Druglike (1)
Label





In [31]:

```
# Show correlation between features using a heatmap
corr = Lipinski[features + ['Target']].corr()
sns.heatmap(corr, annot=True, cmap='coolwarm', fmt=".2f")
plt.title("Feature Correlation Heatmap")
plt.show()
```



	Molecular_Weight	XLogP	H-Bond_Donor_Count	H-Bond_Acceptor_Count	Target
Molecular_Weight	1.00	0.26	0.19	0.61	-0.61
XLogP	0.26	1.00	-0.26	-0.28	-0.03
H-Bond_Donor_Count	0.19	-0.26	1.00	0.37	-0.41
H-Bond_Acceptor_Count	0.61	-0.28	0.37	1.00	-0.69
Target	-0.61	-0.03	-0.41	-0.69	1.00